

Learning Negative Mixture Models by Tensor Decompositions

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Abstract

This work considers the problem of estimating the parameters of *negative mixture models*, i.e. mixture models that possibly involve negative weights. The contributions of this paper are as follows. (i) We show that every rational probability distributions on strings, a representation which occurs naturally in spectral learning, can be computed by a negative mixture of at most two probabilistic automata (or HMMs). (ii) We propose a method to estimate the parameters of negative mixture models having a specific tensor structure in their low order observable moments. Building upon a recent paper on tensor decompositions for learning latent variable models, we extend this work to the broader setting of tensors having a symmetric decomposition with positive *and negative* weights. We introduce a generalization of the *tensor power method* for complex valued tensors, and establish theoretical convergence guarantees. (iii) We show how our approach applies to *negative Gaussian mixture models*, for which we provide some experiments.

Keywords: Spectral learning, Tensor decomposition, Mixture models, Rational series.

1. Introduction

Mixture models, such as Gaussian mixture model, are widely used in statistics and machine learning [Mclachlan and Peel \(2000\)](#). Given a parametric family of probability distributions \mathcal{D} , a mixture is defined by the number of components $k \geq 1$, probabilities $p_1, \dots, p_k \in [0, 1]$ satisfying $p_1 + \dots + p_k = 1$ and distributions F_1, \dots, F_k from \mathcal{D} . Given a sample drawn from a target mixture model, the parameters are usually fit by using the EM algorithm.

Let f_1, \dots, f_k be the PDF associated with F_1, \dots, F_k . It may happen that the function $p_1 f_1 + \dots + p_k f_k$ remains positive even if some of the weights become negative, and still defines a probability density. We call *negative mixtures* such distributions. Only a few papers investigate negative mixtures [Zhang and Zhang \(2005\)](#); [Müller et al. \(2012\)](#); [Jiang et al. \(1999\)](#); [Jevremovic \(1991\)](#). It can easily be seen that every negative mixture can be written as a negative mixture of 2 positive one. We show that negative mixtures naturally occur in spectral learning.

Let Σ be a finite alphabet and let Σ^* denote the set of strings built over Σ . A probability distribution p defined on Σ^* is said to be *rational* if it admits a *linear representation*, i.e. if there exists an integer $n \geq 1$, vectors $\boldsymbol{\iota}, \boldsymbol{\tau} \in \mathbb{R}^n$ and matrices $\mathbf{M}_x \in \mathbb{R}^{n \times n}$ associated with each letter $x \in \Sigma$ such that $p(u_1 \dots u_l) = \boldsymbol{\iota}^\top \mathbf{M}_{u_1} \dots \mathbf{M}_{u_l} \boldsymbol{\tau}$ [Denis and Esposito \(2008\)](#). It can easily be shown that any probability distribution defined by a hidden Markov model (HMM), or equivalently, by a probabilistic automaton, is rational. However, there exist rational probability distributions that cannot be computed by a HMM. The spectral learning algorithms used to infer probability distributions from a sample of strings generally output rational probability distributions. Positive and negative mixtures of rational distributions are rational. Positive mixtures of distributions computed by HMMs can be computed by HMMs. In this paper, we show that every rational distribution p is a negative mixture

$(1+w)p_{H_1} - wp_{H_2}$ of two distributions computed by HMMs. So, negative mixtures occur naturally. How the parameters of the target model can be fit?

In a recent paper, it has been shown that the parameters of a number of latent variable models, including Gaussian mixture models and HMMs, can easily be estimated from tensor decomposition of low-order moments of the data [Anandkumar et al. \(2012\)](#). Typically, if \mathbf{x} is drawn according to the (positive) mixture $p_1\mathcal{N}(\boldsymbol{\mu}_1, \sigma) + \dots + p_k\mathcal{N}(\boldsymbol{\mu}_k, \sigma)$ of spherical Gaussians whose centers $\boldsymbol{\mu}_i$ are linearly independent, the tensors $\mathbf{M}_2 = \sum_{i=1}^k p_i \boldsymbol{\mu}_i \otimes \boldsymbol{\mu}_i$ and $\mathbf{M}_3 = \sum_{i=1}^k p_i \boldsymbol{\mu}_i \otimes \boldsymbol{\mu}_i \otimes \boldsymbol{\mu}_i$ can be expressed as functions of the moments $\mathbb{E}[\mathbf{x} \otimes \mathbf{x}]$ and $\mathbb{E}[\mathbf{x} \otimes \mathbf{x} \otimes \mathbf{x}]$ [Hsu and Kakade \(2013\)](#). Using the fact that \mathbf{M}_2 is positive semidefinite, \mathbf{M}_3 can be reduced to a tensor $\tilde{\mathbf{M}}_3$ admitting an *orthonormal* decomposition $\tilde{\mathbf{M}}_3 = \sum_{i=1}^k \tilde{p}_i \tilde{\boldsymbol{\mu}}_i \otimes \tilde{\boldsymbol{\mu}}_i \otimes \tilde{\boldsymbol{\mu}}_i$, where $\tilde{\boldsymbol{\mu}}_i^\top \tilde{\boldsymbol{\mu}}_j = \delta_{ij}$, and from which the original parameters p_i and $\boldsymbol{\mu}_i$ can be recovered. Lastly, it is shown that a decomposition of an orthogonally decomposable tensor can quickly and robustly be approximated by means of a *tensor power method*. These results induce a learning scheme, which appears as a generalization of the spectral learning approach: from a sample S , compute estimates of \mathbf{M}_2 and \mathbf{M}_3 , compute $\tilde{\mathbf{M}}_3$ and use the tensor power method to compute an orthogonal decomposition of $\tilde{\mathbf{M}}_3$ from which the parameters of the target can be estimated.

Each step of the previous scheme strongly use the facts that the weights p_i are positive and that the $\boldsymbol{\mu}_i$ are linearly independent. We extend it to the case where the weights p_i may be negative. The extension is not straightforward since it needs to use complex square roots of negative real numbers and to introduce non-hermitian quadratic forms.

Given the tensors $\mathbf{M}_2 = \sum_{i=1}^k p_i \boldsymbol{\mu}_i \otimes \boldsymbol{\mu}_i$ and $\mathbf{M}_3 = \sum_{i=1}^k p_i \boldsymbol{\mu}_i \otimes \boldsymbol{\mu}_i \otimes \boldsymbol{\mu}_i$ where the vectors $\boldsymbol{\mu}_i \in \mathbb{R}^n$ are still linearly independent but where the weights p_i may be negative, we first show how \mathbf{M}_3 can be reduced to a complex-valued pseudo-orthonormal decomposable tensor, i.e. of the form $\sum_{i=1}^k \tilde{p}_i \tilde{\boldsymbol{\mu}}_i \otimes \tilde{\boldsymbol{\mu}}_i \otimes \tilde{\boldsymbol{\mu}}_i$, where the vectors $\tilde{\boldsymbol{\mu}}_i \in \mathbb{C}^k$ satisfy $\tilde{\boldsymbol{\mu}}_i^\top \tilde{\boldsymbol{\mu}}_j = \delta_{ij}$ (for any vector $\boldsymbol{\mu} \in \mathbb{C}^k$, $\boldsymbol{\mu}^\top \boldsymbol{\mu} \in \mathbb{C}$ since $\boldsymbol{\mu}^\top$ is **not** the conjugate transpose of $\boldsymbol{\mu}$) and where the weights \tilde{p}_i are non-zero complex numbers. Then, we show how the tensor power method can be adapted to the complex case, with equivalent convergence guarantees. We deduce from these results a learning scheme for negative mixtures. To illustrate this analysis, we experiment our decomposition algorithm on negative mixtures of spherical Gaussian models and we show how estimates of a negative mixture target can be inferred from data.

The paper is organized as follows: preliminaries on rational probability distributions and tensor decomposition learning methods are given in Section 2; negative mixtures are introduced in Section 3 and two introductory examples are developed; the adaptation of the tensor decomposition learning scheme to negative mixtures and the main results of the paper are given in Section 4; an application to negative mixtures of spherical gaussians and some experiments are provided in Sections 5 and 6; a conclusion ends the paper.

2. Preliminaries

2.1. Rational probability distributions on strings

Let Σ be a finite alphabet and Σ^* denote the set of all finite strings built over Σ . A *series* is a mapping $r : \Sigma^* \rightarrow \mathbb{R}$. A non negative series r is *convergent* if the sum $\sum_{w \in \Sigma^*} r(w)$ is bounded; its limit is denoted by $r(\Sigma^*)$. A *probability distribution* over Σ^* is a non-negative series that converges to 1. A series r over Σ is *rational* if there exists an integer $n \geq 1$, two vectors $\boldsymbol{\iota}, \boldsymbol{\tau} \in \mathbb{R}^n$ and a matrix

$\mathbf{M}_x \in \mathbb{R}^{n \times n}$ for each $x \in \Sigma$ such that for all $u = u_1 \dots u_n \in \Sigma^*$, $r(u) = \boldsymbol{\iota}^T \mathbf{M}_{u_1} \dots \mathbf{M}_{u_n} \boldsymbol{\tau}$ [Berstel and Reutenauer \(1988\)](#). The triplet $\langle \boldsymbol{\iota}, (\mathbf{M}_x)_{x \in \Sigma}, \boldsymbol{\tau} \rangle$ is called an n -dimensional *linear representation* of r . An n -states probabilistic automaton (PA) can be defined as an n -dimensional *linear representation* $\langle \boldsymbol{\iota}, (\mathbf{M}_x)_{x \in \Sigma}, \boldsymbol{\tau} \rangle$ whose coefficients are all non-negative and satisfy the following syntactical conditions

$$\boldsymbol{\iota}^T \mathbf{1} = 1, \mathbf{I} - \mathbf{M}_\Sigma \text{ is invertible and } (\mathbf{I} - \mathbf{M}_\Sigma)^{-1} \boldsymbol{\tau} = \mathbf{1}$$

where $\mathbf{1} = (1, \dots, 1)^T \in \mathbb{R}^n$ and $\mathbf{M}_\Sigma = \sum_{x \in \Sigma} \mathbf{M}_x$. Hidden Markov Models (HMM) and PAs define the same probability distributions [Dupont et al. \(2005\)](#). There exist rational probabilistic distributions that cannot be computed by a PA or a HMM (see Appendix A.1).

2.2. Moments method and tensor decomposition

See [Kolda and Bader \(2009\)](#) for references on tensor decomposition. Let us denote by $\bigotimes^p \mathbb{K}^n$ the p -th order tensor product of the vector space \mathbb{K}^n , where $\mathbb{K} = \mathbb{R}$ or \mathbb{C} . A tensor $\mathcal{T} \in \bigotimes^p \mathbb{K}^n$ can be described by a p -way array of scalars $t_{i_1, \dots, i_p} \in \mathbb{K}$ for $i_1, \dots, i_p \in [n]$, where $[n]$ denotes the set of integers between 1 and n . A tensor is *symmetric* if its multi-way array representation is invariant under permutation of the indices. Given $\mathbf{v}^{(1)}, \dots, \mathbf{v}^{(p)} \in \mathbb{K}^n$, the tensor $\mathbf{v}^{(1)} \otimes \dots \otimes \mathbf{v}^{(p)} \in \bigotimes^p \mathbb{K}^n$ is defined by the p -way array $(v_{i_1}^{(1)} v_{i_2}^{(2)} \dots v_{i_p}^{(p)})_{i_1, \dots, i_p \in [n]}$. For a vector $\mathbf{v} \in \mathbb{K}^n$, let $\mathbf{v}^{\otimes p} = \mathbf{v} \otimes \dots \otimes \mathbf{v}$ denote the p -th tensor power of \mathbf{v} . In particular, $\mathbf{v} \otimes \mathbf{v}$ can be identified with the matrix $\mathbf{v} \mathbf{v}^T$. Let \mathbf{x} be a \mathbb{R}^n -valued random variable, its moment of order m is defined as the tensor $\mathbb{E}[\mathbf{x}^{\otimes m}] \in \bigotimes^m \mathbb{R}^n$.

For any integers $m_1, \dots, m_p \geq 1$, every p -th order tensor $\mathcal{T} \in \bigotimes^p \mathbb{K}^n$ induces a multilinear map $\mathcal{T} : \mathbb{K}^{n \times m_1} \times \dots \times \mathbb{K}^{n \times m_p} \rightarrow \mathbb{K}^{m_1 \times \dots \times m_p}$ defined by $\mathcal{T}(\mathbf{A}^{(1)}, \dots, \mathbf{A}^{(p)})_{i_1, \dots, i_p} = \sum_{j_1, \dots, j_p \in [n]} t_{j_1, \dots, j_p} a_{j_1 i_1}^{(1)} \dots a_{j_p i_p}^{(p)}$ where each $i_k \in [m_k]$ for $k \in [p]$. In particular,

$$\text{if } \mathcal{T} = \sum_{i=1}^k \lambda_i \mathbf{v}_i^{(1)} \otimes \dots \otimes \mathbf{v}_i^{(p)} \text{ then } \mathcal{T}(\mathbf{A}_1, \dots, \mathbf{A}_p) = \sum_{i=1}^k \lambda_i (\mathbf{A}_1^T \mathbf{v}_i^{(1)}) \otimes \dots \otimes (\mathbf{A}_p^T \mathbf{v}_i^{(p)}).$$

The *rank* of a tensor $\mathcal{T} \in \bigotimes^p \mathbb{K}^n$ is the smallest integer k such that \mathcal{T} can be written as $\mathcal{T} = \sum_{i=1}^k \lambda_i \mathbf{v}_i^{(1)} \otimes \dots \otimes \mathbf{v}_i^{(p)}$ with $\lambda_i \in \mathbb{K}$ and $\mathbf{v}_i^{(1)}, \dots, \mathbf{v}_i^{(p)} \in \mathbb{K}^n$. The *symmetric rank* of a symmetric tensor \mathcal{T} is the smallest integer k such that \mathcal{T} can be written as $\mathcal{T} = \sum_{i=1}^k \lambda_i \mathbf{v}_i^{\otimes p}$ with $\lambda_i \in \mathbb{K}$ and $\mathbf{v}_i \in \mathbb{K}^n$. It has been shown that computing the rank of a tensor is NP-hard and it is conjectured that computing the symmetric rank is also NP-hard [Hillar and Lim \(2013\)](#). However, if a real-valued third-order tensor \mathcal{T} has a *symmetric orthonormal decomposition*, i.e. $\mathcal{T} = \sum_{i=1}^k \lambda_i \mathbf{v}_i^{\otimes 3}$ with $\lambda_i \in \mathbb{R}$, $\mathbf{v}_i \in \mathbb{R}^n$ and $\mathbf{v}_i^T \mathbf{v}_j = \delta_{ij}$ for all $i, j \in [k]$, it has been shown in [Anandkumar et al. \(2012\)](#) that this decomposition can be recovered by several methods, both efficient and robust to noise, such as the *tensor power method* (see Section 4.2 below). Moreover, they show that any *symmetric independent decomposition* $\mathcal{T} = \sum_{i=1}^k \lambda_i \mathbf{v}_i^{\otimes 3}$ (where the \mathbf{v}_i 's are independent but not necessarily orthonormal) can be recovered if we have access to the second order tensor $\mathbf{M} = \sum_{i=1}^k \lambda_i \mathbf{v}_i \mathbf{v}_i^T$.

Theorem 1 [Anandkumar et al. \(2012\)](#) Let $\mathbf{v}_1, \dots, \mathbf{v}_k$ be linearly independent vectors of \mathbb{R}^n , $\lambda_1, \dots, \lambda_k$ be positive scalars, $\mathbf{M}_2 = \sum_{i=1}^k \lambda_i \mathbf{v}_i \otimes \mathbf{v}_i$ and $\mathcal{M}_3 = \sum_{i=1}^k \lambda_i \mathbf{v}_i^{\otimes 3}$, let $\mathbf{W} \in \mathbb{R}^{n \times k}$ be a matrix such that $\mathbf{M}_2(\mathbf{W}, \mathbf{W}) = \mathbf{I}_k$, the $k \times k$ identity matrix, and let $\boldsymbol{\nu}_i = \sqrt{\lambda_i} \mathbf{W}^T \mathbf{v}_i$ for $i \in [k]$. Then, $\mathcal{M}_3(\mathbf{W}, \mathbf{W}, \mathbf{W}) = \sum_{i=1}^k \lambda_i^{-1/2} \boldsymbol{\nu}_i^{\otimes 3}$ is an orthonormal decomposition from which the parameters λ_i and \mathbf{v}_i can be computed.

2.3. Learning mixtures of spherical Gaussians

The *spherical Gaussian mixture model* is specified as follows: let $k \geq 1$ be the number of components, and for $i \in [n]$, let $p_i > 0$ be the probability of choosing the component $\mathcal{N}(\boldsymbol{\mu}_i, \sigma_i^2 \mathbf{I})$ where $\boldsymbol{\mu}_i \in \mathbb{R}^n$, $\sigma_i^2 > 0$ and $\mathbf{I} \in \mathbb{R}^{n \times n}$ is the identity matrix.

Assuming that the component mean vectors $\boldsymbol{\mu}_i$ are linearly independent, the following result is proved in [Hsu and Kakade \(2013\)](#).

Theorem 2 *The average variance $\bar{\sigma}^2 = \sum_{i=1}^k p_i \sigma_i^2$ is the smallest eigenvalue of the covariance matrix $\mathbb{E}[(\mathbf{x} - \mathbb{E}[\mathbf{x}])(\mathbf{x} - \mathbb{E}[\mathbf{x}])^\top]$. Let \mathbf{v} be any unit-norm eigenvector corresponding to $\bar{\sigma}^2$ and let*

$$\begin{aligned} \mathbf{m}_1 &= \mathbb{E}[\mathbf{x}(\mathbf{v}^\top (\mathbf{x} - \mathbb{E}[\mathbf{x}]))^2], \quad \mathbf{M}_2 = \mathbb{E}[\mathbf{x} \otimes \mathbf{x}] - \bar{\sigma}^2 \mathbf{I}, \quad \text{and} \\ \mathcal{M}_3 &= \mathbb{E}[\mathbf{x} \otimes \mathbf{x} \otimes \mathbf{x}] - \sum_{i=1}^n [\mathbf{m}_1 \otimes \mathbf{e}_i \otimes \mathbf{e}_i + \mathbf{e}_i \otimes \mathbf{m}_1 \otimes \mathbf{e}_i + \mathbf{e}_i \otimes \mathbf{e}_i \otimes \mathbf{m}_1] \end{aligned}$$

where $\mathbf{e}_1, \dots, \mathbf{e}_n$ is the coordinate basis of \mathbb{R}^n . Then,

$$\mathbf{m}_1 = \sum_{i=1}^k p_i \sigma_i^2 \boldsymbol{\mu}_i, \quad \mathbf{M}_2 = \sum_{i=1}^k p_i \boldsymbol{\mu}_i \otimes \boldsymbol{\mu}_i, \quad \text{and} \quad \mathcal{M}_3 = \sum_{i=1}^k p_i \boldsymbol{\mu}_i \otimes \boldsymbol{\mu}_i \otimes \boldsymbol{\mu}_i.$$

The previous results induce a learning scheme: (i) estimate \mathbf{m}_1 , \mathbf{M}_2 and \mathcal{M}_3 from the learning data; (ii) compute an orthonormal decomposition as in Theorem 1; (iii) use the tensor power method to compute the mean vectors $\boldsymbol{\mu}_i$ and the probabilities p_i and (iv) use \mathbf{m}_1 to recover the variance parameters σ_i^2 .

3. Negative mixtures

Given a finite set of probability density functions f_1, \dots, f_k , and non negative weights w_1, \dots, w_k satisfying $w_1 + \dots + w_k = 1$, $w_1 f_1 + \dots + w_k f_k$ is a probability density function called a *finite mixture*. It may happen that $w_1 f_1 + \dots + w_k f_k$ defines a PDF even if some weights are negative. We call such a function a *negative* or a *generalized mixture*.

For example, if f and g are two PDF satisfying $g \leq cf$ for some $c > 1$, then $\alpha f - (\alpha - 1)g$ is a negative mixture for any $0 \leq \alpha - 1 \leq (c - 1)^{-1}$. It can easily be shown, by grouping the positive and negative weights respectively, that any negative mixture can be written as a negative mixture of two positive mixtures:

$$\sum_{i=1}^k \alpha_i f_i - \sum_{j=1}^h \beta_j g_j = A \left(\sum_{i=1}^k \frac{\alpha_i}{A} f_i \right) - B \left(\sum_{j=1}^h \frac{\beta_j}{B} g_j \right)$$

where $\alpha_i, \beta_j > 0$, $A = \sum_{i=1}^k \alpha_i$, $B = \sum_{j=1}^h \beta_j$ and $A - B = 1$.

If f, g and α are known, and if we have access to a random generator \mathcal{D}_f , then Algorithm 1 simulates the distribution $\mathcal{D}_{\alpha f - (\alpha - 1)g}$ by rejection sampling.

Algorithm 1 Simulating a negative mixture

```

drawn  $\leftarrow$  false
while not drawn do
    draw  $x$  according to  $\mathcal{D}_f$ 
    draw  $e$  uniformly in  $[0, 1]$ 
    if  $e\alpha f(x) \geq (\alpha - 1)g(x)$  then
        drawn  $\leftarrow$  true
    end if
end while
return  $x$ 
    
```

3.1. Negative mixtures and rational distributions on strings

We show below that every rational probability distribution on strings can be generated by the generalized mixture of at most two probabilistic automata. The proof relies on the following lemmas.

Lemma 3 *Any rational series is the difference of two rational series with non negative coefficients.*

Proof For any real number x , let $x^+ = \max\{x, 0\}$ and $x^- = \max\{-x, 0\}$. So, $x = x^+ - x^-$. These operators are extended to vectors and matrices by applying them to all their coefficients.

Let $\langle \iota, (\mathbf{M}_x)_{x \in \Sigma}, \tau \rangle$ be an n -dimensional representation of a rational series r . Let us define

$$\tilde{\iota}_1 = \begin{pmatrix} \iota^+ \\ \iota^- \end{pmatrix}, \tilde{\iota}_2 = \begin{pmatrix} \iota^- \\ \iota^+ \end{pmatrix}, \tilde{\tau} = \begin{pmatrix} \tau^+ \\ \tau^- \end{pmatrix} \text{ and } \widetilde{\mathbf{M}}_x = \begin{pmatrix} \mathbf{M}_x^+ & \mathbf{M}_x^- \\ \mathbf{M}_x^- & \mathbf{M}_x^+ \end{pmatrix} \text{ for each } x \in \Sigma.$$

Let r^+ (resp. r^-) be the rational series defined by the linear representation $\langle \tilde{\iota}_1, (\widetilde{\mathbf{M}}_x)_{x \in \Sigma}, \tilde{\tau} \rangle$ (resp. $\langle \tilde{\iota}_2, (\widetilde{\mathbf{M}}_x)_{x \in \Sigma}, \tilde{\tau} \rangle$). Then, $r = r^+ - r^-$. Indeed, it can easily be checked that for any vectors $\mathbf{u}_1, \mathbf{u}_2, \mathbf{v}_1, \mathbf{v}_2 \in \mathbb{R}^n$,

$$\widetilde{\mathbf{M}}_x \begin{pmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \end{pmatrix} = \begin{pmatrix} \mathbf{v}_1 \\ \mathbf{v}_2 \end{pmatrix} \Rightarrow \mathbf{M}_x(\mathbf{u}_1 - \mathbf{u}_2) = \mathbf{v}_1 - \mathbf{v}_2.$$

Therefore, for any $w = w_1 \dots w_n \in \Sigma^*$,

$$\widetilde{\mathbf{M}}_{w_1} \dots \widetilde{\mathbf{M}}_{w_n} \tilde{\tau} = \begin{pmatrix} \mathbf{v}_1 \\ \mathbf{v}_2 \end{pmatrix} \Rightarrow \mathbf{M}_{w_1} \dots \mathbf{M}_{w_n} \tau = \mathbf{v}_1 - \mathbf{v}_2.$$

Since

$$(\tilde{\iota}_1^\top - \tilde{\iota}_2^\top) \begin{pmatrix} \mathbf{v}_1 \\ \mathbf{v}_2 \end{pmatrix} = \iota^\top (\mathbf{v}_1 - \mathbf{v}_2),$$

it can easily be checked that

$$r^+(w) - r^-(w) = (\tilde{\iota}_1^\top - \tilde{\iota}_2^\top) \widetilde{\mathbf{M}}_{w_1} \dots \widetilde{\mathbf{M}}_{w_n} \tilde{\tau} = r(w).$$

■

However, even if the non negative series r is convergent, the series r^+ and r^- obtained from the previous construction can be divergent (see an example in Appendix A.1). It has been shown in Bailly

and Denis (2011) that if a rational series r is absolutely convergent, then it can always be computed by a linear representation $\langle \iota, (\mathbf{M}_x)_{x \in \Sigma}, \tau \rangle$ such that $\langle |\iota|, (|\mathbf{M}_x|)_{x \in \Sigma}, |\tau| \rangle$ defines a positive convergent series s . In that case, r^+ and r^- are bounded by s and are convergent. Let $s^+ = r^+(\Sigma^*)$, $s^- = r^-(\Sigma^*)$ and let $p^+ = r^+/s^+$ and $p^- = r^-/s^-$: p^+ and p^- are rational probability distributions and if r is itself a probability distribution, we have $s^+ - s^- = 1$ and r is equal to the generalized mixture $s^+p^+ - s^-p^-$. It remains to prove that p^+ and p^- can be computed by a probabilistic automaton.

Lemma 4 *Let $\langle \iota, (\mathbf{M}_x)_{x \in \Sigma}, \tau \rangle$ be an n -dimensional minimal non negative linear representation of a probability distribution p . Let $\lambda = (\mathbf{I} - \mathbf{M}_\Sigma)^{-1}\tau$ and $\mathbf{D} = \text{diag}(\lambda)$.*

Then, $\langle \mathbf{D}\iota, (\mathbf{D}^{-1}\mathbf{M}_x\mathbf{D})_{x \in \Sigma}, \mathbf{D}^{-1}\tau \rangle$ is a probabilistic automaton that recognizes p .

Proof The minimality of the representation implies that \mathbf{D} is invertible. It is clear that the new representation recognizes p since $(\mathbf{D}\iota)^\top \mathbf{D}^{-1}\mathbf{M}_{x_1}\mathbf{D} \dots \mathbf{D}^{-1}\mathbf{M}_{x_n}\mathbf{D} \mathbf{D}^{-1}\tau = \iota^\top \mathbf{M}_{x_1} \dots \mathbf{M}_{x_n} \tau$. We have $(\mathbf{D}\iota)^\top \mathbf{1} = \iota^\top \lambda = 1$. Moreover, $\mathbf{I} - \mathbf{D}^{-1}\mathbf{M}_\Sigma\mathbf{D} = \mathbf{D}^{-1}(\mathbf{I} - \mathbf{M}_\Sigma)\mathbf{D}$ is invertible and $(\mathbf{I} - \mathbf{D}^{-1}\mathbf{M}_\Sigma\mathbf{D})^{-1}\mathbf{D}^{-1}\tau = \mathbf{D}^{-1}\lambda = 1$. ■

Combining the previous lemmas, we obtain the following theorem.

Theorem 5 *Every rational probability distribution on strings can be generated by the generalized mixture of at most two probabilistic automata.*

3.2. Negative mixtures and gaussians

Let f and g be the PDF of the two k -dimensional Gaussian distributions $\mathcal{N}(\mu_f, \Sigma_f)$ and $\mathcal{N}(\mu_g, \Sigma_g)$.

For any real number $\alpha > 0$,

$$\alpha f(\mathbf{x}) - (\alpha - 1)g(\mathbf{x}) \geq 0 \quad (1)$$

if and only if

$$\exp \left\{ -\frac{1}{2}(\mathbf{x} - \mu_f)^\top \Sigma_f^{-1}(\mathbf{x} - \mu_f) + \frac{1}{2}(\mathbf{x} - \mu_g)^\top \Sigma_g^{-1}(\mathbf{x} - \mu_g) \right\} \geq \sqrt{\frac{|\Sigma_f|}{|\Sigma_g|}} [1 - 1/\alpha].$$

There exists $\alpha > 1$ such that (1) holds for any $\mathbf{x} \in \mathbb{R}^k$ if and only if

$$-(\mathbf{x} - \mu_f)^\top \Sigma_f^{-1}(\mathbf{x} - \mu_f) + (\mathbf{x} - \mu_g)^\top \Sigma_g^{-1}(\mathbf{x} - \mu_g) \quad (2)$$

has a finite lower bound which holds if and only if $(\Sigma_g^{-1} - \Sigma_f^{-1})$ is positive semi-definite.

In that case, the minimum m of (2) is attained for

$$\mu_0 = \Sigma_0(\Sigma_g^{-1}\mu_g - \Sigma_f^{-1}\mu_f)$$

where $\Sigma_0 = (\Sigma_g^{-1} - \Sigma_f^{-1})^{-1}$, and there exists a constant λ such that $\lambda g/f$ defines a Gaussian distribution of parameters μ_0 and Σ_0 . It can be checked that

$$m = -(\mu_f - \mu_g)^\top \Sigma_f^{-1} \Sigma_0 \Sigma_g^{-1} (\mu_f - \mu_g).$$

Note that if the two distributions are distinct, then $\left(\frac{|\Sigma_g|}{|\Sigma_f|}\right)^{1/2} e^{m/2} - 1 < 0$. Otherwise, any positive α would be suitable and by dividing (1) by α , the density of the first distribution would be everywhere larger than the density of the second, which cannot happen. Hence every

$$\alpha \in \left] 1, \left(1 - \sqrt{\frac{|\Sigma_g|}{|\Sigma_f|}} e^{m/2} \right)^{-1} \right]$$

defines a valid negative mixture of the two distributions.

If the gaussians are spherical, i.e. $\Sigma_f = \sigma_f^2 \mathbf{I}$ and $\Sigma_g = \sigma_g^2 \mathbf{I}$, we obtain the following result.

Proposition 6 $\alpha f(\mathbf{x}) - (\alpha - 1)g(\mathbf{x})$ defines a negative mixture iff

$$\sigma_f > \sigma_g \text{ and } 1 < \alpha \leq \left(1 - \frac{\sigma_g^k}{\sigma_f^k} \exp \left\{ -\frac{1}{2} \frac{\|\boldsymbol{\mu}_f - \boldsymbol{\mu}_g\|^2}{\sigma_f^2 - \sigma_g^2} \right\} \right)^{-1}.$$

Example Let $k = 2$, $\boldsymbol{\mu}_f = (11.4 \quad -3.4)^\top$, $\sigma_f^2 = 8$, $\boldsymbol{\mu}_g = (11.9 \quad -1.9)^\top$, $\sigma_g^2 = 4$: $\alpha f(\mathbf{x}) - (\alpha - 1)g(\mathbf{x})$ defines a negative mixture for any $1 < \alpha \leq 1.57$. See figure 1.

4. Negative Mixtures and the Power Method

We consider systems of the form

$$\mathbf{M}_2 = \sum_{i=1}^k w_i \boldsymbol{\mu}_i \otimes \boldsymbol{\mu}_i \quad \text{and} \quad \mathcal{M}_3 = \sum_{i=1}^k w_i \boldsymbol{\mu}_i \otimes \boldsymbol{\mu}_i \otimes \boldsymbol{\mu}_i \quad (3)$$

where the vectors $\boldsymbol{\mu}_1, \dots, \boldsymbol{\mu}_k \in \mathbb{R}^d$ are linearly independent and $w_1, \dots, w_k \in \mathbb{R}$ are non zero.

In this section, we show how the parameters w_i and $\boldsymbol{\mu}_i$ can be recovered from \mathbf{M}_2 and \mathcal{M}_3 using a *power method for complex-valued tensors*.

4.1. Pseudo-Orthonormalization

A set $\{\boldsymbol{\nu}_1, \dots, \boldsymbol{\nu}_k\} \subset \mathbb{C}^d$ is *pseudo-orthonormal* iff $\boldsymbol{\nu}_i^\top \boldsymbol{\nu}_j = \delta_{ij}$ for all $i, j \in [k]$. Note that for any $\boldsymbol{\nu} = (\nu_1, \dots, \nu_d) \in \mathbb{C}^d$, $\boldsymbol{\nu}^\top \boldsymbol{\nu} = \nu_1^2 + \dots + \nu_d^2 \in \mathbb{C}$ and in particular, $\boldsymbol{\nu}^\top \boldsymbol{\nu} \neq \|\boldsymbol{\nu}\|_2^2 = |\nu_1|^2 + \dots + |\nu_d|^2$. It can easily be checked that a pseudo-orthonormal set is linearly independent. A tensor decomposition $\mathcal{T} = \sum_{i=1}^k z_i \boldsymbol{\nu}_i^{\otimes p}$ of a complex-valued tensor $\mathcal{T} \in \bigotimes^p \mathbb{C}^n$ is *pseudo-orthonormal* if $\{\boldsymbol{\nu}_1, \dots, \boldsymbol{\nu}_k\}$ is a pseudo-orthonormal set.

As in Anandkumar et al. (2012), we build a whitening matrix \mathbf{W} from \mathbf{M}_2 , and we use \mathbf{W} to obtain a pseudo-orthonormal decomposition of the tensor \mathcal{M}_3 .

Identifying \mathbf{M}_2 with the symmetric rank- k matrix $\sum_{i=1}^k w_i \boldsymbol{\mu}_i \boldsymbol{\mu}_i^\top$, let $\mathbf{U} \mathbf{D} \mathbf{U}^\top$ be the eigendecomposition of \mathbf{M}_2 , where \mathbf{D} is the $k \times k$ diagonal matrix whose diagonal elements are composed of the k non-zero eigenvalues of \mathbf{M}_2 and where \mathbf{U} is a $d \times k$ matrix satisfying $\mathbf{U}^\top \mathbf{U} = \mathbf{I}_k$ and $\mathbf{U} \mathbf{U}^\top \boldsymbol{\mu}_i = \boldsymbol{\mu}_i$ for any $i \in [k]$. Let $\mathbf{W} = \mathbf{U} \mathbf{D}^{-\frac{1}{2}} \in \mathbb{C}^{d \times k}$ and $\tilde{\boldsymbol{\mu}}_i = w_i^{\frac{1}{2}} \mathbf{W}^\top \boldsymbol{\mu}_i \in \mathbb{C}^k$ for $i \in [k]$ where we consider complex square roots of the negative components of \mathbf{D} and w_i : $x^{1/2} = i|x|^{1/2}$ and $x^{-1/2} = (x^{1/2})^{-1} = -i|x|^{-1/2}$ if $x < 0$. We have

$$\sum_{i=1}^k \tilde{\boldsymbol{\mu}}_i \tilde{\boldsymbol{\mu}}_i^\top = \mathbf{W}^\top \left(\sum_{i=1}^k w_i \boldsymbol{\mu}_i \boldsymbol{\mu}_i^\top \right) \mathbf{W} = \mathbf{W}^\top \mathbf{M}_2 \mathbf{W} = \mathbf{I}_k$$

hence $\widetilde{\boldsymbol{\mu}}_i^\top \widetilde{\boldsymbol{\mu}}_j = \delta_{ij}$ for all $i, j \in [k]$. Now let $\widetilde{\mathcal{M}}_3 = \mathcal{M}_3(\mathbf{W}, \mathbf{W}, \mathbf{W}) = \sum_{i=1}^k w_i (\mathbf{W}^\top \boldsymbol{\mu}_i)^{\otimes 3} = \sum_{i=1}^k w_i^{-\frac{1}{2}} \widetilde{\boldsymbol{\mu}}_i^{\otimes 3}$ which is a pseudo-orthonormal decomposition.

4.2. Power Method for Complex-Valued Tensors

The following theorem extends Lemma 5.1 of [Anandkumar et al. \(2012\)](#) to third-order complex-valued tensors having a pseudo-orthonormal decomposition $\mathcal{T} = \sum_{i=1}^k z_i \boldsymbol{\nu}_i^{\otimes 3}$. Note that the parameters of such a decomposition are not fully identifiable since $z \boldsymbol{\nu}^{\otimes 3} = (-z)(-\boldsymbol{\nu})^{\otimes 3}$.

Theorem 7 *Let $\mathcal{T} \in \otimes^3 \mathbb{C}^n$ have a pseudo-orthonormal decomposition $\mathcal{T} = \sum_{i=1}^k z_i \boldsymbol{\nu}_i^{\otimes 3}$, and let T be the mapping defined by $T(\boldsymbol{\theta}) = \mathcal{T}(I, \boldsymbol{\theta}, \boldsymbol{\theta})$ for any $\boldsymbol{\theta} \in \mathbb{C}^n$. Let $\boldsymbol{\theta}_0 \in \mathbb{C}^n$, suppose that $|z_1 \cdot \boldsymbol{\nu}_1^\top \boldsymbol{\theta}_0| > |z_2 \cdot \boldsymbol{\nu}_2^\top \boldsymbol{\theta}_0| \geq \dots \geq |z_k \cdot \boldsymbol{\nu}_k^\top \boldsymbol{\theta}_0| > 0$. For $t = 1, 2, \dots$, define*

$$\boldsymbol{\theta}_t = \frac{T(\boldsymbol{\theta}_{t-1})}{[T(\boldsymbol{\theta}_{t-1})^\top T(\boldsymbol{\theta}_{t-1})]^\frac{1}{2}} \quad \text{and} \quad \lambda_t = \mathcal{T}(\boldsymbol{\theta}_t, \boldsymbol{\theta}_t, \boldsymbol{\theta}_t) \quad (4)$$

where we assume that $\boldsymbol{\theta}_0$ is such that $T(\boldsymbol{\theta}_t)^\top T(\boldsymbol{\theta}_t) \neq 0$ for all t . Then, $\boldsymbol{\theta}_t \rightarrow \pm \boldsymbol{\nu}_1$ and $\lambda_t \rightarrow \pm z_1$. More precisely, let

$$M = \max \left\{ 1, \frac{|z_1|^2}{|z_i|^2}, |z_1| \frac{\|\boldsymbol{\nu}_i\|}{|z_i|} : i \in [k] \right\} \quad \text{and} \quad \varepsilon_t = kM \left| \frac{z_2 \cdot \boldsymbol{\nu}_2^\top \boldsymbol{\theta}_0}{z_1 \cdot \boldsymbol{\nu}_1^\top \boldsymbol{\theta}_0} \right|^{2^t}.$$

Then for all $t \geq 2$ such that $\varepsilon_t < \frac{1}{2}$, we have

$$|e_t f_t \lambda_t - z_1| \leq 7|z_1| \varepsilon_t \quad \text{and} \quad \|e_t f_t \boldsymbol{\theta}_t - \boldsymbol{\nu}_1\| \leq \varepsilon_t \left(\|\boldsymbol{\nu}_1\| + \sqrt{2} \right),$$

where $(e_t)_t$ and $(f_t)_t$ are two sequences defined in the proof and taking their values in $\{-1, 1\}$.

Proof Let us first define the square root of a complex number $z = r e^{i\theta}$, where $-\pi < \theta \leq \pi$ and $r \geq 0$, by $z^{1/2} = r^{1/2} e^{i\frac{\theta}{2}}$, and note that $z/(z^2)^{1/2} = z^{-1}(z^2)^{1/2} = 1$ if $-\pi/2 < \theta \leq \pi/2$ and -1 otherwise.

Now, let $c_i = \boldsymbol{\nu}_i^\top \boldsymbol{\theta}_0$ for $i \in [k]$, $\widetilde{\boldsymbol{\theta}}_0 = \boldsymbol{\theta}_0$, $\widetilde{\boldsymbol{\theta}}_t = T(\widetilde{\boldsymbol{\theta}}_{t-1})$, and $\rho_t = (\widetilde{\boldsymbol{\theta}}_t^\top \widetilde{\boldsymbol{\theta}}_t)^{\frac{1}{2}}$ for all $t \geq 1$. Check by induction on t that, for all $t \geq 1$,

$$\widetilde{\boldsymbol{\theta}}_t = \sum_{i=1}^k z_i^{2^t-1} c_i^{2^t} \boldsymbol{\nu}_i \quad (5)$$

Let $e_t = \rho_{t+1} \rho_t^{-2} / (\rho_t^{-4} \rho_{t+1}^2)^{\frac{1}{2}}$, note that $e_t = \pm 1$, and check by induction that, for all $t \geq 2$,

$$\boldsymbol{\theta}_t = e_t \frac{\widetilde{\boldsymbol{\theta}}_t}{\rho_t}. \quad (6)$$

Let $\alpha_t = \rho_t^{-1} z_1^{2^t-1} c_1^{2^t}$. Using Eq. 5 and Eq. 6, we obtain

$$\begin{aligned} e_t \lambda_t &= \rho_t^{-3} \sum_{i=1}^k z_i (z_i^{2^t-1} c_i^{2^t})^3 = \alpha_t^3 \sum_{i=1}^k \frac{z_1^3}{z_i^2} \left(\frac{z_i c_i}{z_1 c_1} \right)^{3 \cdot 2^t} = \alpha_t^3 z_1 \left[1 + \sum_{i=2}^k \frac{z_1^2}{z_i^2} \left(\frac{z_i c_i}{z_1 c_1} \right)^{3 \cdot 2^t} \right], \quad \text{and} \\ e_t \boldsymbol{\theta}_t &= \rho_t^{-1} \sum_{i=1}^k z_i^{2^t-1} c_i^{2^t} \boldsymbol{\nu}_i = \alpha_t \sum_{i=1}^k \frac{z_1}{z_i} \left(\frac{z_i c_i}{z_1 c_1} \right)^{2^t} \boldsymbol{\nu}_i = \alpha_t \left[\boldsymbol{\nu}_1 + \sum_{i=2}^k \frac{z_1}{z_i} \left(\frac{z_i c_i}{z_1 c_1} \right)^{2^t} \boldsymbol{\nu}_i \right]. \end{aligned}$$

It can easily be checked that

$$\left| \sum_{i=2}^k \frac{z_1^2}{z_i^2} \left(\frac{z_i c_i}{z_1 c_1} \right)^{3 \cdot 2^t} \right| \leq \varepsilon_t \quad \text{and} \quad \left\| \sum_{i=2}^k \frac{z_1}{z_i} \left(\frac{z_i c_i}{z_1 c_1} \right)^{2^t} \boldsymbol{\nu}_i \right\| \leq \varepsilon_t.$$

Moreover, it can be checked that

$$\alpha_t^{-1} = \frac{(\tilde{\boldsymbol{\theta}}_t^\top \tilde{\boldsymbol{\theta}}_t)^{1/2}}{z_1^{2^t-1} c_1^{2^t}} = f_t \left(\frac{\tilde{\boldsymbol{\theta}}_t^\top \tilde{\boldsymbol{\theta}}_t}{(z_1^{2^t-1} c_1^{2^t})^2} \right)^{1/2} = f_t \left[1 + \sum_{i=2}^k \frac{z_1^2}{z_i^2} \left(\frac{z_i c_i}{z_1 c_1} \right)^{2^{t+1}} \right]^{1/2}$$

where $f_t = (z_1^{2^t-1} c_1^{2^t})^{-1} \left((z_1^{2^t-1} c_1^{2^t})^2 \right)^{\frac{1}{2}} = \pm 1$. Using the hypothesis $\varepsilon_t < \frac{1}{2}$ and making use of Lemma 11 in Appendix A.2, it follows that

$$|\alpha_t| \leq \sqrt{2}, \quad |f_t \alpha_t - 1| \leq \varepsilon_t \quad \text{and} \quad |f_t \alpha_t^3 - 1| \leq 4\varepsilon_t.$$

Finally, combining these inequalities, we obtain

$$|e_t f_t \lambda_t - z_1| \leq 7|z_1| \varepsilon_t \quad \text{and} \quad \|e_t f_t \boldsymbol{\theta}_t - \boldsymbol{\nu}_1\| \leq \varepsilon_t \left(\|\boldsymbol{\nu}_1\| + \sqrt{2} \right).$$

■

This theorem directly yields an algorithm to recover the decomposition of a decomposable complex-valued tensor using the standard deflation technique.

It can be shown that if $\boldsymbol{\theta}_0$ is chosen at random in \mathbb{C}^n , the assumptions on $\boldsymbol{\theta}_t$ in the previous theorem are satisfied with probability one. We prove it here for the assumption $T(\boldsymbol{\theta}_t)^\top T(\boldsymbol{\theta}_t) \neq 0$, similar arguments can be used for the assumption $|z_1 \cdot \boldsymbol{\nu}_1^\top \boldsymbol{\theta}_0| > |z_2 \cdot \boldsymbol{\nu}_2^\top \boldsymbol{\theta}_0| \geq \dots \geq |z_k \cdot \boldsymbol{\nu}_k^\top \boldsymbol{\theta}_0| > 0$.

Lemma 8 *Using the definitions and under the hypothesis of Theorem 7, the set $S = \{\boldsymbol{\theta}_0 \in \mathbb{C}^n | \exists t \geq 0 : T(\boldsymbol{\theta}_t)^\top T(\boldsymbol{\theta}_t) = 0\}$ has Lebesgue measure zero in \mathbb{C}^n .*

Proof We use the notations of the previous proof.

First note that $T(\boldsymbol{\theta}_{t-1})^\top T(\boldsymbol{\theta}_{t-1}) = \left(\tilde{\boldsymbol{\theta}}_{t-1}^\top \tilde{\boldsymbol{\theta}}_{t-1} \right)^{-2} \tilde{\boldsymbol{\theta}}_t^\top \tilde{\boldsymbol{\theta}}_t$ and $\tilde{\boldsymbol{\theta}}_t^\top \tilde{\boldsymbol{\theta}}_t = \sum_{i=1}^k (z_i^{2^t-1} (\boldsymbol{\nu}_i^\top \boldsymbol{\theta}_0)^{2^t})^2$. For a fixed t , the set

$$S_t = \left\{ \boldsymbol{\theta} \in \mathbb{C}^n : P_t(\boldsymbol{\theta}) = \sum_{i=1}^k (z_i^{2^t-1} (\boldsymbol{\nu}_i^\top \boldsymbol{\theta})^{2^t})^2 = 0 \right\}$$

is the set of zeros of a multivariate polynomial. If P_t is non-trivial (i.e. different from zero), it is a proper algebraic subvariety of \mathbb{C}^n of dimension less than n , thus of Lebesgue measure 0. Since $S = \cup_{t=0}^\infty S_t$, it is sufficient to show that P_t is non-trivial for any index t .

Without loss of generality, we assume that there exists at least one $i \in [k]$ such that the first component $\nu_{i,1}$ of the vector $\boldsymbol{\nu}_i$ is not null. Suppose that P_t is null, then all of its monomials are null. In particular, the coefficient associated with $\theta_1^{2^{t+1}-1} \theta_j$, which is proportional to $\sum_{i=1}^k z_i^{2^{t+1}-2} \nu_{i,1}^{2^{t+1}-1} \nu_{i,j}$, is null for all $j \in [n]$. Let $\alpha_i = z_i^{2^{t+1}-2} \nu_{i,1}^{2^{t+1}-1}$ for $i \in [k]$, and note that

since $z_i \neq 0$ for all $i \in [k]$, we cannot have all the α_i equal to zero. Thus, we have $\sum_i \alpha_i \nu_{i,j} = 0$ for all $j \in [n]$, i.e. $\sum_{i=1}^k \alpha_i \nu_i = \mathbf{0}$ which is in contradiction with the linear independence of $\{\nu_i\}_{i=1}^k$. \blacksquare

We can now state the following theorem, which summarizes the overall procedure to recover the parameters of a system of the form (3) using pseudo-orthonormalization and the complex tensor power method. Note that this procedure generalizes the one proposed in Anandkumar et al. (2012): if all the weights w_1, \dots, w_k are positive, the method we propose boils down to theirs.

Theorem 9 *Let $\mu_1, \dots, \mu_k \in \mathbb{R}^n$ be linearly independent, $w_1, \dots, w_k \neq 0 \in \mathbb{R}$, $\mathbf{M}_2 = \sum_{i=1}^k w_i \mu_i \otimes \mu_i$ and $\mathcal{M}_3 = \sum_{i=1}^k w_i \mu_i \otimes \mu_i \otimes \mu_i$. Let $\mathbf{U}\mathbf{D}\mathbf{U}^\top$ be the eigendecomposition of \mathbf{M}_2 , $\mathbf{W} = \mathbf{U}\mathbf{D}^{-\frac{1}{2}} \in \mathbb{C}^{n \times k}$ (see section 4.1) and $(\mathbf{W}^\top)^+ = \mathbf{U}\mathbf{D}^{\frac{1}{2}}$. Finally, let $\mathcal{T} = \mathcal{M}_3(\mathbf{W}, \mathbf{W}, \mathbf{W})$ and let θ_0 be drawn at random in \mathbb{C}^k .*

Then, using the definitions of θ_t and λ_t in Eq. 4, we have

$$\lim_t \frac{1}{\lambda_t^2} = w_j \quad \text{and} \quad \lim_t \lambda_t (\mathbf{W}^\top)^+ \theta_t = \mu_j$$

with probability one, where $j = \arg \max_i \{|\mu_i^\top \mathbf{W} \theta_0|\}$.

The indeterminacy on the sign of the coefficients in the pseudo-orthogonal decomposition $\mathcal{T} = \sum_{i=1}^k w_i^{-\frac{1}{2}} \left(w_i^{\frac{1}{2}} \mathbf{W}^\top \mu_i \right)^{\otimes 3}$ vanishes when we recover the original parameters w_i and μ_i .

5. Learning Negative Mixtures of Spherical Gaussians

In this section, we extend the method described in Section 2.3 to estimate the parameters of a negative mixture of spherical Gaussians. Let $f(\mathbf{x}) = \sum_{i=1}^k w_i \mathcal{N}(\mathbf{x}; \mu_i, \sigma_i^2 \mathbf{I})$ be the PDF of the random vector \mathbf{x} , where $\mu_i \in \mathbb{R}^n$ are the component means, σ_i^2 the component variances, and $w_i \neq 0$ the coefficients ($\sum_{i=1}^k w_i = 1$). Assuming that the component means are linearly independent, we have the following result which generalizes Theorem 2.

Theorem 10 *The average variance $\bar{\sigma}^2 = \sum_{i=1}^k w_i \sigma_i^2$ is an eigenvalue of the covariance matrix $\mathbb{E}[(\mathbf{x} - \mathbb{E}[\mathbf{x}])(\mathbf{x} - \mathbb{E}[\mathbf{x}])^\top]$. Let \mathbf{v} be any unit-norm eigenvector corresponding to $\bar{\sigma}^2$. We have $\mathbf{m}_1 = \sum_{i=1}^k w_i \sigma_i^2 \mu_i$, $\mathbf{M}_2 = \sum_{i=1}^k w_i \mu_i \otimes \mu_i$, and $\mathcal{M}_3 = \sum_{i=1}^k w_i \mu_i \otimes \mu_i \otimes \mu_i$, where \mathbf{m}_1 , \mathbf{M}_2 and \mathcal{M}_3 are defined as in Theorem 2.*

Moreover, let r be the number of negative eigenvalues of the matrix $\mathbf{M} = \sum_{i=1}^k w_i (\mu_i - \mathbb{E}[\mathbf{x}]) \otimes (\mu_i - \mathbb{E}[\mathbf{x}])$. Then $\bar{\sigma}^2$ is the $(r+1)$ -th smallest eigenvalue of the covariance matrix.

The proof of this theorem is given in Appendix A.3, where we also show that $r = l$ or $l+1$, where l is the number of negative coefficients w_i , i.e. $l = |\{w_i : i \in [k], w_i < 0\}|$.

This theorem, combined with Theorem 9, yields a procedure to estimate the parameters of a negative mixture of spherical Gaussians: (i) compute the sample covariance matrix \mathbf{S} , (ii) for each candidate eigenvalue of \mathbf{S} for $\bar{\sigma}^2$, estimate the tensors \mathbf{m}_1 , \mathbf{M}_2 and \mathcal{M}_3 on the data, (iii) compute estimations of the parameters using Algorithm 2, (iv) choose the model that maximizes the likelihood of the learning data.

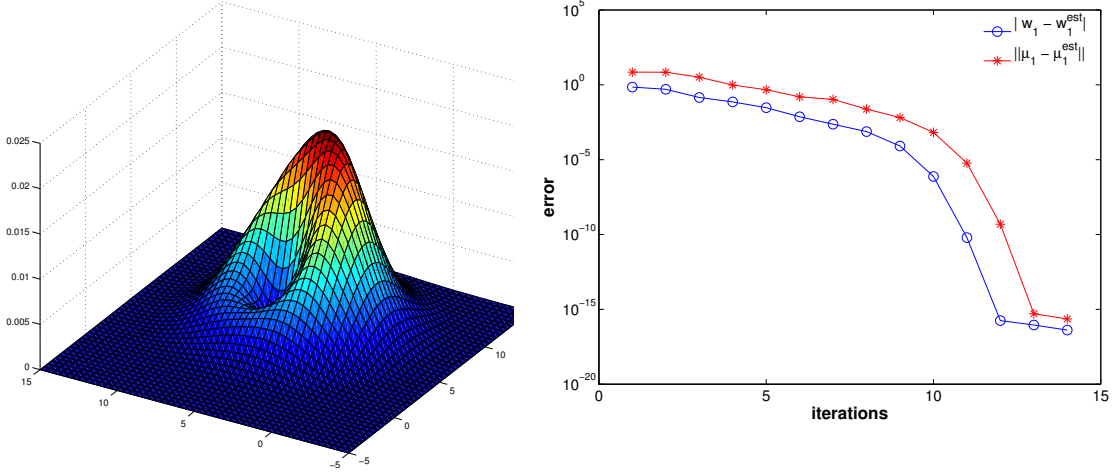


Figure 1: (left) Density function of a negative mixture of spherical Gaussians with parameters $w_1 = 1.5$, $\boldsymbol{\mu}_1 = (11.4 \ -3.4)^\top$, $\sigma_1^2 = 8$, $w_2 = -0.5$, $\boldsymbol{\mu}_2 = (11.9 \ -1.9)^\top$ and $\sigma_2^2 = 4$. (right) Convergence rate of the proposed method on the exact tensors \mathbf{M}_2 and \mathbf{M}_3 .

6. Experiments

We illustrate the results presented above on the running example defined in Figure 1 (left). The algorithm to estimate the parameters of a system of the form (3) from estimation of the tensors \mathbf{M}_2 and \mathbf{M}_3 is summarized in Figure 2 (left).

First, we run Algorithm 2 on the exact tensors $\mathbf{M}_2 = \sum_{i=1}^k w_i \boldsymbol{\mu}_i \otimes \boldsymbol{\mu}_i$ and $\mathbf{M}_3 = \sum_{i=1}^k w_i \boldsymbol{\mu}_i \otimes \boldsymbol{\mu}_i \otimes \boldsymbol{\mu}_i$ with various initializations of $\boldsymbol{\theta}_0$ to extract the first eigenvector/eigenvalue pair. The corresponding parameters w_i and $\boldsymbol{\mu}_i$ are always exactly recovered in less than 15 iterations, the average error over 500 initializations for those two parameters in function of the number of iterations is plotted in Figure 1 (right).

Then, we test our algorithm in a learning setting. For various sizes (ranging from 1,000 to 400,000), we generate 100 datasets (using Algorithm 1) and use the method described in the previous section to estimate the parameters of the negative mixture of Gaussians. The results are plotted in Figure 2 (right), where each point represents the average on the 100 datasets of the l^2 -norm between the true parameters ($\mathbf{U} = [\boldsymbol{\mu}_1 \ \boldsymbol{\mu}_2]$ and $\mathbf{w} = [w_1 \ w_2]$) and the estimations.

For some of these datasets, our algorithm returns a decomposition involving complex valued vectors and weights; for the experiments, we only used the real parts in the error measure. The number of these pathological datasets decreases toward zero as their size increases.

Algorithm 2 Negative Mixture Estimation

Input: $k \in \mathbb{N}$, $\widehat{\mathbf{M}}_2 \in \bigotimes^2 \mathbb{R}^n$, $\widehat{\mathbf{M}}_3 \in \bigotimes^3 \mathbb{R}^n$

Output: $w_1, \dots, w_k, \mu_1, \dots, \mu_k$

$\mathbf{U}\mathbf{D}\mathbf{U}^\top \leftarrow \widehat{\mathbf{M}}_2$ (k -truncated eig. decomp.);

$\mathbf{W} \leftarrow \mathbf{U}\mathbf{D}^{-\frac{1}{2}}$; $\mathcal{T} \leftarrow \widehat{\mathbf{M}}_3(\mathbf{W}, \mathbf{W}, \mathbf{W})$;

for $i = 1$ **to** k **do**

 Draw θ at random in \mathbb{C}^k ;

repeat

$\theta \leftarrow \mathcal{T}(I, \theta, \theta)$; $\theta \leftarrow \frac{\theta}{(\theta^\top \theta)^{\frac{1}{2}}}$;

until stabilization

$\lambda \leftarrow \mathcal{T}(\theta, \theta, \theta)$; $\mathcal{T} \leftarrow \mathcal{T} - \lambda \cdot \theta^{\otimes 3}$;

$w_i \leftarrow 1/\lambda^2$; $\mu_i \leftarrow \lambda(\mathbf{W}^\top)^+ \theta$;

end for

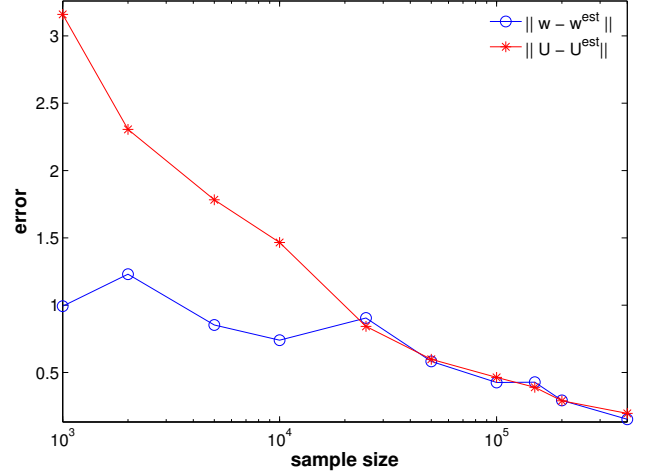


Figure 2: (left) Algorithm for the estimation of the parameters of a negative mixture model from estimation of the low-order moment tensors.
(right) Estimation error as a function of the dataset size.

7. Conclusion

In this paper, we propose a first introductory study of negative mixture models. We argue that these models may appear naturally in several learning settings — such as spectral learning of probability distributions on strings — when the learning schemes rely on algebraic methods applied without positivity constraints (i.e. on fields, e.g. \mathbb{R} , rather than semi-fields, e.g. \mathbb{R}_+).

These models may seem difficult to handle, since allowing negative weights exclude the use of probabilistic methods such as EM. However, tensor decomposition techniques can be an appealing alternative. The complex tensor power method we propose, along with its application to the negative Gaussian mixture model, is a first step toward a deep understanding of these models and the elaboration of tools to use them.

This work could be extended in several ways. First, other fields of machine learning where negative mixture models appear, or where their expressiveness can be useful, should be investigated. By extending the power method to complex valued tensors, we are able to propose an algorithm to estimate the parameters of such models, but the implications of using decomposition techniques on complex tensors need to be studied further. In particular, a deep robustness analysis of our method would help to understand its behavior in the learning setting.

References

- Anima Anandkumar, Rong Ge, Daniel Hsu, Sham M. Kakade, and Matus Telgarsky. Tensor decompositions for learning latent variable models. *CoRR*, abs/1210.7559, 2012.
- Raphaël Bailly and François Denis. Absolute convergence of rational series is semi-decidable. *Inf. Comput.*, 209(3):280–295, 2011.
- Jean Berstel and Christophe Reutenauer. *Rational series and their languages*. EATCS monographs on theoretical computer science. Springer-Verlag, Berlin, New York, 1988. ISBN 0-387-18626-3. URL <http://opac.inria.fr/record=b1086956>. Translation of: Les sries rationnelles et leurs langages.
- François Denis and Yann Esposito. On rational stochastic languages. *Fundam. Inform.*, 86(1-2): 41–77, 2008.
- S. W. Dharmadhikari. Sufficient conditions for a stationary process to be a function of a finite markov chain. *Ann. Math. Statist.*, pages 1033–1041, 1963.
- Pierre Dupont, François Denis, and Yann Esposito. Links between probabilistic automata and hidden markov models: probability distributions, learning models and induction algorithms. *Pattern Recognition*, 38(9):1349–1371, 2005.
- Christopher J. Hillar and Lek-Heng Lim. Most tensor problems are NP-hard. *J. ACM*, 60(6):45:1–45:39, November 2013. ISSN 0004-5411. doi: 10.1145/2512329. URL <http://doi.acm.org/10.1145/2512329>.
- Daniel Hsu and Sham M. Kakade. Learning mixtures of spherical gaussians: Moment methods and spectral decompositions. In *Proceedings of the 4th Conference on Innovations in Theoretical Computer Science*, ITCS ’13, pages 11–20, New York, NY, USA, 2013. ACM. ISBN 978-1-4503-1859-4. doi: 10.1145/2422436.2422439. URL <http://doi.acm.org/10.1145/2422436.2422439>.
- Vesna Jevremovic. A note on mixed exponential distribution with negative weights. *Statistics & Probability Letters*, 11(3):259–265, March 1991. URL <http://www.sciencedirect.com/science/article/B6V1D-45FCH7X-19/1/d619b073faa264427eb090e5f4b1159d>.
- R. Jiang, M.J. Zuo, and H.-X. Li. Weibull and inverse weibull mixture models allowing negative weights. *Reliability Engineering & System Safety*, 66(3):227 – 234, 1999. ISSN 0951-8320. doi: [http://dx.doi.org/10.1016/S0951-8320\(99\)00037-X](http://dx.doi.org/10.1016/S0951-8320(99)00037-X). URL <http://www.sciencedirect.com/science/article/pii/S095183209900037X>.
- Tamara G. Kolda and Brett W. Bader. Tensor decompositions and applications. *SIAM REVIEW*, 51(3):455–500, 2009.
- Geoffrey McLachlan and David Peel. *Finite Mixture Models*. Wiley Series in Probability and Statistics. Wiley-Interscience, 2000. URL <http://www.amazon.com/exec/obidos/redirect?tag=citeulike07-20&path=ASIN/0471006262>.

Philipp Müller, Simo Ali-LyTTY, Marzieh Dashti, Henri Nurminen, and Robert Pich. Gaussian mixture filter allowing negative weights and its application to positioning using signal strength measurements. In *WPNC*, pages 71–76. IEEE, 2012. ISBN 978-1-4673-1437-4. URL <http://dblp.uni-trier.de/db/conf/wpnc/wpnc2012.html#MullerADNP12>.

Petra Perner and Atsushi Imiya, editors. *Machine Learning and Data Mining in Pattern Recognition, 4th International Conference, MLDM 2005, Leipzig, Germany, July 9-11, 2005, Proceedings*, volume 3587 of *Lecture Notes in Computer Science*, 2005. Springer. ISBN 3-540-26923-1.

Baibo Zhang and Changshui Zhang. Finite mixture models with negative components. In [Perner and Imiya \(2005\)](#), pages 31–41. ISBN 3-540-26923-1.

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Appendix A. Proofs and Complements

A.1. Rational probability distributions on strings

Probabilistic automatas and HMMs define the same family of probability distributions on strings [Dupont et al. \(2005\)](#). All these distributions are rational but the converse is false [Dharmadhikari \(1963\)](#); [Denis and Esposito \(2008\)](#). The simplest counter examples can be built on a one-letter alphabet and a dimension equal to 3.

Let $\Sigma = \{a\}$ be a one-letter alphabet. Let us define a parametrized family of linear representations by

$$\iota = (\lambda, 0, \sqrt{2}\lambda)^\top, M = \rho \begin{pmatrix} \cos \alpha & -\sin \alpha & 0 \\ \sin \alpha & \cos \alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tau = (1, 1, 1)^\top$$

where $\lambda > 0$ and $0 < \rho < 1$. Let r be the associated rational series. It can easily be seen that

$$r(a^n) = \rho^n \sqrt{2}\lambda [\cos(n\alpha - \pi/4) + 1] \geq 0$$

for all n . We have also

$$r(\Sigma^*) = \lambda \left[\frac{1 - \sqrt{2}\rho \cos(\alpha - \pi/4)}{1 + \rho^2 - 2\rho \cos \alpha} + \frac{\sqrt{2}}{1 - \rho} \right]$$

and λ can always be chosen such that $r(\Sigma^*) = 1$, i.e. such that r is a probability distribution. It can easily be seen that r can be defined by a PA iff $\alpha/\pi \in \mathbb{Q}$.

For example, if $\cos \alpha = 3/5$, $\sin \alpha = 4/5$, the corresponding distributions cannot be computed by a PA.

If $\rho = 0.5$, we have $\lambda = \frac{13}{6+26\sqrt{2}}$ and $\boldsymbol{\iota} \simeq (0.304, 0, 0.430)^\top$. The construction described in Section 3.1 yields the distributions p^+ and p^- respectively defined by the following PAs:

$$\boldsymbol{\iota}^+ = (0.4015, 0, 0.5985, 0, 0)^\top, \mathbf{M}^+ = \begin{pmatrix} 0.300 & 0 & 0 & 0 & 0.173 \\ 0.302 & 0.3 & 0 & 0 & 0 \\ 0 & 0 & 0.5 & 0 & 0 \\ 0 & 0.7 & 0 & 0.3 & 0 \\ 0 & 0 & 0 & 0.7 & 0.300 \end{pmatrix}, \boldsymbol{\tau}^+ = (0.527, 0.398, 0.5, 0, 0)^\top,$$

$$\boldsymbol{\iota}^- = (0, 0, 1, 0)^\top, \mathbf{M}^- = \begin{pmatrix} 0.300 & 0 & 0 & 0.173 \\ 0.302 & 0.3 & 0 & 0 \\ 0 & 0.7 & 0.3 & 0 \\ 0 & 0 & 0.7 & 0.300 \end{pmatrix}, \boldsymbol{\tau}^- = (0.527, 0.398, 0, 0)^\top,$$

and the mixture parameters $s^+ = 1.4364$ and $s^- = -0.4364$.

If $\rho = 0.75$, the series r^+ and r^- computed by Lemma 3 do not converge. It is necessary to compute first a linear representation $(\boldsymbol{\iota}, \mathbf{M}, \boldsymbol{\tau})$ of r such that the series associated with $(|\boldsymbol{\iota}|, |\mathbf{M}|, |\boldsymbol{\tau}|)$ is convergent. This can be achieved using techniques described in Bailly and Denis (2011). For example, we obtain the following linear representation

$$\boldsymbol{\iota} = (1, 0, 0, 0, 0, 0)^\top, M = \begin{pmatrix} 0 & 0.5675 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.7125 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.9566 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.9753 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.8334 \\ 0.5662 & -0.1571 & 0 & 0 & 0 & 0.2750 \end{pmatrix},$$

and $\boldsymbol{\tau} = (0.43250, 0.2875, 0.0434, 0.0247, 0.1666, 0.3159)^\top$ from which the construction described in Section 3.1 can be applied.

A.2. Proof of Lemma 11

Lemma 11 *Let $k > 0$ and $z \in \mathbb{C}$ such that $|z| < 1/2$. Then,*

$$|(1+z)^{-k} - 1| \leq 2|z|(2^k - 1).$$

In particular,

$$|(1+z)^{-1/2} - 1| \leq |z| \text{ and } |(1+z)^{-3/2} - 1| \leq 4|z|.$$

Proof Let $f(z) = (1+z)^{-k} - 1$ with $k > 0$ and $|z| < 1/2$; $f'(z) = -k(1+z)^{-(k+1)}$. Let $\gamma : [0, 1] \mapsto \mathbb{C}$ s.t. $\gamma(t) = tz$. We have

$$\begin{aligned} (1+z)^{-k} - 1 &= \int_{\gamma} f'(y) dy = \int_0^1 f'(\gamma(t)) \gamma'(t) dt \\ &= -kz \int_0^1 (1+tz)^{-(k+1)} dt. \end{aligned}$$

Therefore,

$$\begin{aligned} |(1+z)^{-k} - 1| &\leq k|z| \int_0^1 (1-t|z|)^{-(k+1)} dt \\ &= [(1-t|z|)^{-k}]_0^1 = (1-|z|)^{-k} - 1 \\ &\leq 2|z|(2^k - 1). \end{aligned}$$

Indeed, let $g(x) = (1 - x)^{-k} - 1 - 2x(2^k - 1)$. It can be checked that $g(0) = g(1/2) = 0$ and that g is convex on $[0, 1/2]$. ■

A.3. Proof of Theorem 10

We will need the following results. The first one is a corollary of the *Sylvester's Law of Inertia*.

Lemma 12 *Let $\mathbf{Q} \in \mathbb{R}^{n \times n}$ be a symmetric real matrix. Suppose that there exists a non singular matrix $\mathbf{P} \in \mathbb{R}^{n \times n}$ and $w_1, \dots, w_n \in \mathbb{R}$ such that $\mathbf{Q} = \mathbf{P}^\top \mathbf{D} \mathbf{P}$ where $\mathbf{D} = \text{diag}(w_1, \dots, w_n)$, the diagonal matrix whose diagonal entries are w_1, \dots, w_n . Then, the number of negative eigenvalues of \mathbf{Q} is equal to the number of negative coefficients w_i .*

Lemma 13 (Weyl's Inequality) *Let \mathbf{A} and \mathbf{B} be two $n \times n$ hermitian matrices. We have $\sigma_1(\mathbf{A}) + \sigma_i(\mathbf{B}) \leq \sigma_i(\mathbf{A} + \mathbf{B}) \leq \sigma_n(\mathbf{A}) + \sigma_i(\mathbf{B})$ for all $i \in [n]$, where $\sigma_i(\mathbf{M})$ denotes the i -th smallest eigenvalue of \mathbf{M} .*

Lemma 14 *Let $\{\mathbf{v}_i\}_{i=1}^k$ be a linearly dependent family of vectors of \mathbb{R}^n , where $n \geq k$, such that any of its subset of size $k - 1$ is linearly independent. We consider the rank $k - 1$ matrix $\mathbf{M} = \sum_{i=1}^k w_i \mathbf{v}_i \mathbf{v}_i^\top$ where $w_1, \dots, w_k \neq 0$. Let l be the number of negative coefficients w_i . Then the first null eigenvalue of \mathbf{M} is either the l -th or the $(l + 1)$ -th smallest one.*

Proof If $l = 0$, then \mathbf{M} is positive semi-definite and $\sigma_1(\mathbf{M}) = 0$. If $l = k$, then \mathbf{M} is negative semi-definite and $\sigma_k(\mathbf{M}) = 0$.

We suppose that $1 \leq l \leq k - 1$.

For $1 \leq j \leq k$, let $\mathbf{M}_j = \sum_{1 \leq i \neq j \leq k} w_i \mathbf{v}_i \mathbf{v}_i^\top$ and l_j be the number of negative coefficients in $\{w_i\}_{1 \leq i \neq j \leq k}$. Let V_j be the vector space spanned by $\{\mathbf{v}_1, \dots, \bar{\mathbf{v}}_j, \dots, \mathbf{v}_k\}$, where the notation $\bar{\mathbf{v}}_j$ means that \mathbf{v}_j is omitted. Let $\boldsymbol{\nu}_k, \dots, \boldsymbol{\nu}_n$ be a linearly independent family of vectors in V_j^\perp and \mathbf{P} be the non singular $n \times n$ matrix $[\mathbf{v}_1 \dots, \bar{\mathbf{v}}_j, \dots, \mathbf{v}_k, \boldsymbol{\nu}_k, \dots, \boldsymbol{\nu}_n]^\top$. Clearly,

$$\mathbf{M}_j = \mathbf{P}^\top \text{diag}(w_1, \dots, \bar{w}_j, \dots, w_k, 0, \dots, 0) \mathbf{P}$$

and therefore, from Lemma 12, l_j is the number of negative eigenvalues of \mathbf{M}_j .

For any $j \in [k]$, we consider the decomposition $\mathbf{M} = w_j \mathbf{v}_j \mathbf{v}_j^\top + \mathbf{M}_j$, sum of two hermitian matrices. The first summand is a rank one matrix whose only non null eigenvalue has the same sign as w_j , and the second has $k - 1$ non zero eigenvalues, among l_j are negative.

Let j be an index such that $w_j < 0$: from Weil's inequality $\sigma_i(\mathbf{M}) \leq 0 + \sigma_i(\mathbf{M}_j)$ for any $i \in [n]$. Since \mathbf{M}_j has $l_j = l - 1$ negative eigenvalues, \mathbf{M} has at least $l - 1$ negative eigenvalues.

Let j be an index such that $w_j > 0$: Weil's inequality gives $\sigma_i(\mathbf{M}) \geq 0 + \sigma_i(\mathbf{M}_j)$ for any $i \in [n]$, thus \mathbf{M} has at least $k - l - 1$ positive eigenvalues, hence at most l negative ones.

Therefore, the first null eigenvalue of \mathbf{M} must be either the l -th or the $(l + 1)$ -th smallest one. ■

Let $f(\mathbf{x}) = \sum_{i=1}^k w_i \mathcal{N}(\mathbf{x}; \boldsymbol{\mu}_i, \sigma_i^2 \mathbf{I})$ be the PDF of the random vector \mathbf{x} , and let l be the number of negative weights w_i . We can now prove Theorem 10, along with the relation between l and the position of the eigenvalue $\bar{\sigma}^2$ in the covariance matrix.

Theorem *The average variance $\bar{\sigma}^2 = \sum_{i=1}^k w_i \sigma_i^2$ is an eigenvalue of the covariance matrix $\mathbb{E}[(\mathbf{x} - \mathbb{E}[\mathbf{x}])(\mathbf{x} - \mathbb{E}[\mathbf{x}])^\top]$. Let \mathbf{v} be any unit-norm eigenvector corresponding to $\bar{\sigma}^2$. We have $\mathbf{m}_1 = \sum_{i=1}^k w_i \sigma_i^2 \boldsymbol{\mu}_i$, $\mathbf{M}_2 = \sum_{i=1}^k w_i \boldsymbol{\mu}_i \otimes \boldsymbol{\mu}_i$, and $\mathbf{M}_3 = \sum_{i=1}^k w_i \boldsymbol{\mu}_i \otimes \boldsymbol{\mu}_i \otimes \boldsymbol{\mu}_i$, where \mathbf{m}_1 , \mathbf{M}_2 and \mathbf{M}_3 are defined as in Theorem 2.*

Moreover, let r be the number of negative eigenvalues of the matrix $\mathbf{M} = \sum_{i=1}^k w_i (\boldsymbol{\mu}_i - \mathbb{E}[\mathbf{x}]) \otimes (\boldsymbol{\mu}_i - \mathbb{E}[\mathbf{x}])$. Then $\bar{\sigma}^2$ is the $(r+1)$ -th smallest eigenvalue of the covariance matrix.

Furthermore, r is either equal to l or $l+1$.

Proof Most of the proof of this theorem for usual Gaussian mixtures in Hsu and Kakade (2013) relies on the introduction of a discrete latent variable h : the sampling process is interpreted as first sampling h with $\mathbb{P}[h = i] = w_i$, and then sampling $\mathbf{x} = \boldsymbol{\mu}_h + \mathbf{z}_h$ where \mathbf{z}_h is a multivariate Gaussian with mean $\mathbf{0}$ and covariance $\sigma_h^2 \mathbf{I}$. Allowing negative weights in the mixture, we cannot use the same strategy, but it will be sufficient to note that $\mathbb{E}[g(\mathbf{x})] = \sum_{i=1}^k w_i \mathbb{E}[g(\boldsymbol{\mu}_i + \mathbf{z}_i)]$ for any function g , which is a direct consequence of the linearity of the expectation.

First, we need to identify the position of $\bar{\sigma}^2$ in the covariance matrix. Let $\bar{\boldsymbol{\mu}} = \mathbb{E}[\mathbf{x}] = \sum_{i=1}^k w_i \boldsymbol{\mu}_i$. The covariance matrix of \mathbf{x} is

$$\mathbb{E}[(\mathbf{x} - \bar{\boldsymbol{\mu}}) \otimes (\mathbf{x} - \bar{\boldsymbol{\mu}})] = \sum_{i=1}^k w_i (\boldsymbol{\mu}_i - \bar{\boldsymbol{\mu}}) \otimes (\boldsymbol{\mu}_i - \bar{\boldsymbol{\mu}}) + \bar{\sigma}^2 \mathbf{I}.$$

Since the $\boldsymbol{\mu}_i$'s are linearly independent, $F = \{\boldsymbol{\mu}_i - \bar{\boldsymbol{\mu}}\}_{i=1}^k$ is a linearly dependent family of vectors of \mathbb{R}^n such that any of its subset of size $k-1$ is linearly independent. It follows from Lemma 14 that 0 is either the l -th or $(l+1)$ -th smallest eigenvalue of the matrix $\sum_{i=1}^k w_i (\boldsymbol{\mu}_i - \bar{\boldsymbol{\mu}}) \otimes (\boldsymbol{\mu}_i - \bar{\boldsymbol{\mu}})$, which implies that $\bar{\sigma}^2$ is the corresponding eigenvalue in the covariance matrix.

Note that the strict separation of $\bar{\sigma}^2$ from the other eigenvalues in the covariance matrix implies that every eigenvector corresponding to $\bar{\sigma}^2$ is in the null space of $\sum_{i=1}^k w_i (\boldsymbol{\mu}_i - \bar{\boldsymbol{\mu}}) \otimes (\boldsymbol{\mu}_i - \bar{\boldsymbol{\mu}})$, hence $\mathbf{v}^\top (\boldsymbol{\mu}_i - \bar{\boldsymbol{\mu}}) = 0$ for all $i \in [k]$.

We now express \mathbf{m}_1 , \mathbf{M}_2 and \mathbf{M}_3 in terms of the parameters w_i , σ_i^2 and $\boldsymbol{\mu}_i$. First,

$$\begin{aligned} \mathbf{m}_1 &= \mathbb{E}[\mathbf{x}(\mathbf{v}^\top (\mathbf{x} - \mathbb{E}[\mathbf{x}]))^2] \\ &= \sum_{i=1}^k w_i \mathbb{E}[(\boldsymbol{\mu}_i + \mathbf{z}_i)(\mathbf{v}^\top (\boldsymbol{\mu}_i - \bar{\boldsymbol{\mu}} + \mathbf{z}_i))^2] \\ &= \sum_{i=1}^k w_i \mathbb{E}[(\boldsymbol{\mu}_i + \mathbf{z}_i)(\mathbf{v}^\top \mathbf{z}_i)^2] = \sum_{i=1}^k w_i \sigma_i^2 \boldsymbol{\mu}_i. \end{aligned}$$

Next, since $\mathbb{E}[\mathbf{z}_i \otimes \mathbf{z}_i] = \sigma_i^2 \mathbf{I}$ for all $i \in [k]$, we have

$$\begin{aligned} \mathbf{M}_2 &= \mathbb{E}[\mathbf{x} \otimes \mathbf{x}] - \bar{\sigma}^2 \mathbf{I} \\ &= \sum_{i=1}^k w_i \mathbb{E}[(\boldsymbol{\mu}_i + \mathbf{z}_i) \otimes (\boldsymbol{\mu}_i + \mathbf{z}_i)] - \bar{\sigma}^2 \mathbf{I} \\ &= \sum_{i=1}^k w_i (\boldsymbol{\mu}_i \otimes \boldsymbol{\mu}_i + \mathbb{E}[\mathbf{z}_i \otimes \mathbf{z}_i]) - \bar{\sigma}^2 \mathbf{I} = \sum_{i=1}^k w_i \boldsymbol{\mu}_i \otimes \boldsymbol{\mu}_i. \end{aligned}$$

Finally, writing z_{ij} for the j -th component of the vector \mathbf{z}_i , we have

$$\begin{aligned} \sum_{i=1}^k w_i \mathbb{E}[\boldsymbol{\mu}_i \otimes \mathbf{z}_i \otimes \mathbf{z}_i] &= \sum_{i=1}^k w_i \sum_{p=1}^n \sum_{q=1}^n \mathbb{E}[z_{ip} z_{iq}] \boldsymbol{\mu}_i \otimes \mathbf{e}_p \otimes \mathbf{e}_q \\ &= \sum_{i=1}^k w_i \sigma_i^2 \sum_{j=1}^n \boldsymbol{\mu}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_j \\ &= \sum_{j=1}^n \mathbf{m}_1 \otimes \mathbf{e}_j \otimes \mathbf{e}_j, \end{aligned}$$

where we used the fact that $\mathbb{E}[z_{ip} z_{iq}] = \delta_{pq} \sigma_i^2$ for all $i \in [k]$, $p, q \in [n]$. Using the same derivation, we have $\sum_{i=1}^k w_i \mathbb{E}[\mathbf{z}_i \otimes \boldsymbol{\mu}_i \otimes \mathbf{z}_i] = \sum_{j=1}^n \mathbf{e}_j \otimes \mathbf{m}_1 \otimes \mathbf{e}_j$ and $\sum_{i=1}^k w_i \mathbb{E}[\mathbf{z}_i \otimes \mathbf{z}_i \otimes \boldsymbol{\mu}_i] = \sum_{j=1}^n \mathbf{e}_j \otimes \mathbf{e}_j \otimes \mathbf{m}_1$. Hence,

$$\begin{aligned} \mathbb{E}[\mathbf{x}^{\otimes 3}] &= \sum_{i=1}^k w_i (\boldsymbol{\mu}_i^{\otimes 3} + \mathbb{E}[\boldsymbol{\mu}_i \otimes \mathbf{z}_i \otimes \mathbf{z}_i] + \mathbb{E}[\mathbf{z}_i \otimes \boldsymbol{\mu}_i \otimes \mathbf{z}_i] + \mathbb{E}[\mathbf{z}_i \otimes \mathbf{z}_i \otimes \boldsymbol{\mu}_i]) \\ &= \sum_{i=1}^k w_i \boldsymbol{\mu}_i^{\otimes 3} + \sum_{j=1}^n (\mathbf{m}_1 \otimes \mathbf{e}_j \otimes \mathbf{e}_j + \mathbf{e}_j \otimes \mathbf{m}_1 \otimes \mathbf{e}_j + \mathbf{e}_j \otimes \mathbf{e}_j \otimes \mathbf{m}_1) \end{aligned}$$

and $\mathcal{M}_3 = \sum_{i=1}^k w_i \boldsymbol{\mu}_i \otimes \boldsymbol{\mu}_i \otimes \boldsymbol{\mu}_i$. ■